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Foreword

One of the most amazing facts about nature is how the fundamental particles combine into three basic building blocks—the proton, neutron and electron—under the conditions found on earth. Equally amazing is that these three particles can be aggregated into a hundred or so formations, called atoms, that form the basis of life and nature as we know it. As we aggregate atoms into molecules and compounds, the number of possible combinations becomes infinite, yet the regularity persists. This regularity of construction is marvelous, yet taken for granted.

Function follows form, and the function and properties of compounds are determined by their structure. Crystallography is the study of the structure of regular solid-state substances, and its importance is hard to overestimate. Crystallography was one of the first scientific disciplines to computerize, thereby allowing the determination of simple structures to become straightforward and of complicated structures to be possible. A natural consequence of using the computer to generate data was to use it to archive data already generated. Crystallography and neutron physics were in fact among the first areas to create numerical scientific databases. Over the last 40 years, the importance of crystallographic database work has grown enormously. Virtually all structure determinations have been archived in databases which allow easy access and complete coverage. Thousands of scientists all over the world successfully use these databases on a daily basis for a wide variety of applications.

Today, the computer revolution continues: new processors allow computations of a scale impossible just 15 years ago; database technology makes data storage and retrieval easy; and the internet makes data access trivial. How do these developments affect existing crystallographic data activities, which have evolved into a coordinated, comprehensive set of separate activities? What are the new demands that the scientific community is placing on the crystallographic data activities now that materials design from first principles is becoming a reality? Finally, what new efforts are needed to enhance the data activities, perhaps having them become more integrated? Questions such as these made it timely to organize this workshop on the crystallographic databases and to have a frank and open discussion amongst the representatives of the data activities with input from users. The reader will find in these pages not only a review of all existing crystallographic data activities, but also some answers to the questions just raised.

The NIST Standard Reference Data Program has long supported many crystallographic data efforts and is very interested in promoting discussions on issues related to the collection, evaluation, and dissemination of crystallographic data. Dr. Mary Good, Under Secretary of Technology in the U.S. Department of Commerce, joins me in thanking Vicky Lynn Karen and Alan Mighell of the NIST Crystal and Electron Diffraction Data Center for organizing the workshop and pulling together these proceedings. Opportunities for growth in terms of the nature and scope of new data activities and greater cooperation have been identified. We all look forward to further progress in meeting the need to preserve and access data on one of nature's most marvelous creations: the regularity of the structure of matter.

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